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Semiclassical Theory of Positron Emission in Transient Supercritical Atoms

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Within the semiclassical approximation (WKB) we present an estimate of the cross section for spontaneous and induced positron emission during the formation of a supercritical atom in a heavy-ion collision. Energy and width of the electron levels are taken from an analytical WKB formula.

1. Introduction

It is known [1–3] that the $1s_{1/2}$ electron energy reaches the top of the negative energy continuum for the critical nuclear charge $Z_{cr} \approx 170$. By expanding the electronic wave function around Z_{cr} it has been shown [4, 5] that the $1s_{1/2}$ level dives into the continuum for $Z > Z_{cr}$ but remains localized in space.

The degeneracy of the $1s_{1/2}$ level with the negative continuum leads to electronic transitions from the negative continuum into the $1s_{1/2}$ state if the latter is vacant. The resulting holes in the continuum escape as free positrons. The rate of this spontaneous positron emission depends on the width of the $1s_{1/2}$ level [6, 7].

Supercritical atoms ($Z > Z_{cr}$) can be produced in heavy-ion collisions only. The sum of the nuclear charges of target (Z_T) and projectile (Z_P) must exceed Z_{cr}. Then, at a critical internuclear distance R_{cr} the $1s\sigma_g$ level of the temporarily formed molecule reaches $E = -mc^2$. For a U – U molecule, R_{cr} is estimated to lie between 34 and 51 fm [7, 8]. In close collisions at sufficiently high ion energies, $R < R_{cr}$ is possible and spontaneous emission of positrons will take place, provided there is a K-shell vacancy in the molecule.

Collisions between very heavy ions and atoms whose relative velocity is nonrelativistic will always be adiabatic with respect to the motion of the inner shell electrons. However, nonadiabatic effects play an important role. An electronic transition from the negative continuum into the $1s\sigma_g$ state can be induced by the time variation of the potential between molecule and electron. This induced positron emission [9] does not require degeneracy of the two states, and it can occur for an arbitrary R.

It is the purpose of this paper to derive the positron decay rates within the semiclassical approximation, which are valid for any Z, not only for the region of low supercriticality as assumed in References 8 and 9. Our discussion emphasizes the physical ideas of the semiclassical method in connection with positron emission, and it leads to simple analytical formulas.

We calculate in Section 2 the energy and the width of the $1s_{1/2}$ level in supercritical atoms from the resonant behaviour of the phase shift [10], applying the WKB approximation. In Section 3 the cross section for the spontaneous positron emission is discussed.

Starting from an adiabatic basis we derive in Section 4 an estimate for the induced positron emission cross section.

2. Energy and Width of the K-shell in Supercritical Atoms

A K-shell vacancy in a nucleus with $Z > Z_{cr}$ is unstable against pair creation. From the definition of the vacuum as the state of minimum energy [11] it follows that an empty bound state in the negative continuum represents a quasibound positron. This positron can escape by tunneling through a potential

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barrier. As has been pointed out by Zeldovich and Popov [3], this barrier comes from the effective, energy-dependent potential of a Schrödinger-like equation into which the single-particle Dirac equation can be transformed. Although the barrier appears for all s states with negative energy their width, i.e. the tunneling probability, is non-zero in the supercritical region only ($E < -mc^2$).

2.1. Wave Function

In the case of s states the WKB approximation should also be reliable. We insert

$$F = a\exp(iS/\hbar); \quad G = b\exp(iS/\hbar) \tag{2.1}$$

into the radial Dirac equation where $F(r)/r$ stands for the large and $G(r)/r$ for the small component of the $1s_{1/2}$ state:

$$(E - mc^2 - V)F + \hbar c G' + \hbar c/r\, G = 0$$
$$(E + mc^2 - V)G - \hbar c F' + \hbar c/r\, F = 0. \tag{2.2}$$

If only zero order terms in $\hbar$ are considered one finds

$$S' \equiv p = [(E - mc^2 - V)(E + mc^2 - V)]^{1/2}/c$$
$$\equiv [2m(W - U)]^{1/2} \tag{2.3}$$

with $W = (E^2 - m^2c^4)/2mc^2$ the effective energy, and $U = (EV - V^2/2)/mc^2$ the effective potential. By reason of simplicity the nuclear potential V is chosen to be constant inside the nucleus with radius R_0

$$V(r) = \begin{cases} -Ze^2/r, & r > R_0 \\ -Ze^2/R_0, & r \leq R_0. \end{cases}$$

For this case Figure 1 shows the effective potential $U(r)$ together with the two classical turning points.
From the boundary condition $F = G = 0$ at $r = 0$ we obtain in WKB approximation

$$F = a_1 \sin\left(\hbar^{-1}\int_0^r p\,dr\right) \Big/ (pc)^{1/2} \tag{2.4}$$

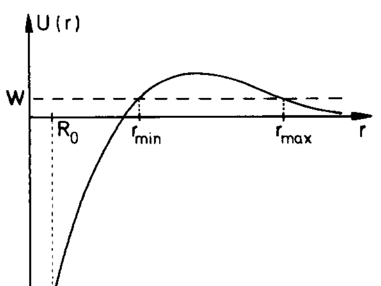

Fig. 1. Effective potential $U(r)$ and effective energy W for the Coulomb problem with $Z > 170$

valid for $r \leq r_{\min} = Ze^2/(mc^2 - E)$. In the barrier region $r_{\min} < r < r_{\max} = -Ze^2/(mc^2 + E)$ we have

$$F = a_1/2 \exp\left(i\pi/4 - \hbar^{-1}\int_{r_{\min}}^{r} |p|\,dr\right) \Big/ (|p|c)^{1/2}.$$

The constant a_1 follows from normalization. The small component is given by

$$G = i[(E - mc^2 - V)/(E + mc^2 - V)]^{1/2} F. \tag{2.5}$$

For vanishing potential the WKB solution (2.4) goes over into the exact free solution of the Dirac equation. It therefore is an exact solution in the nuclear interior for the cut-off potential defined above.

2.2. Energy

The shape of the effective potential implies that there are bound states in the continuum which can decay via tunneling through the barrier into free states of the negative continuum. This means that the quasi-stationary bound states appear as resonances in the scattering phase shift. These resonances were obtained [10] from a phase shift analysis of the exact negative continuum solutions of the Dirac equation in a supercritical field.
In WKB approximation the calculation becomes very simple. One starts from the semiclassical expression for that part of the phase shift which is relevant to the resonance [12]

$$\delta_1 = -\arctan[1/4\, T^2 \cot(\phi - \pi/2)], \tag{2.6}$$

where T is the tunneling amplitude

$$T = \exp\left(-\hbar^{-1}\int_{r_{\min}}^{r_{\max}} |p|\,dr\right) \tag{2.7}$$

and ϕ is the classical action

$$\phi = \hbar^{-1}\int_0^{r_{\min}} p\,dr. \tag{2.8}$$

As usual, the energies E_n result from the poles of $\cot(\phi - \pi/2)$:

$$\phi = \pi(n + 1/2) \tag{2.9}$$

with $n = 1, 2, \ldots$ the principal quantum number. From this condition together with (2.8) and (2.3) one obtains the eigenvalue equation

$$(mc^2)^{1/2}/(\hbar c\pi)\left\{ba^{-1/2}/2\ln\frac{2ar_{\min} + b}{2(al)^{1/2} + 2aR_0 + b}\right.$$
$$\left. - d^{1/2}\ln\frac{2d/r_{\min} + b}{2(dl)^{1/2}/R_0 + 2d/R_0 + b}\right\}$$
$$= n + 1/2 \tag{2.10}$$

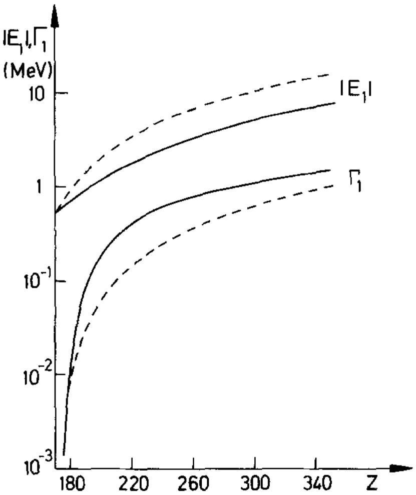

Fig. 2. Energy and width of the $1s_{1/2}$ state in the WKB approximation. Full lines without, broken lines with centrifugal potential

with

$$a=2W;\quad b=2Ze^2E/mc^2;\quad R_0=r_0 Z^{1/3};$$
$$d=Z^2e^4/mc^2;\quad l=aR_0^2+bR_0+d.$$

The parameter r_0 is taken to be 1.425 fm so that $E_{n=1}=-mc^2$ for $Z=Z_{cr}=170$.
In the nonrelativistic limit one must replace $n+1/2$ by n in order to obtain the hydrogen energy. The reason for this change of quantization is that the nuclear potential remains finite when r goes to zero, which is essential for $Z \geqq 137$ but not for $Z<137$.
The $1s_{1/2}$ eigenvalues E_1 are shown in Figure 2 as a function of Z.

2.3. Decay Width

By expanding ϕ around the eigenvalue E_n one obtains the well known Breit-Wigner denominator $(E_n-E)-i\Gamma_n/2$ for the scattering amplitude. The width Γ_n of the resonance is given by [12]

$$\Gamma_n=T^2(E_n)\Big/\left(2\frac{\partial\phi}{\partial E}(E_n)\right). \tag{2.11}$$

With (2.7) and (2.8) we obtain for the cut-off Coulomb potential

$$\frac{\partial\phi}{\partial E}=\tau E/(2\hbar mc^2)+Ze^2/(\hbar c(mc^2)^{1/2})$$
$$\cdot\left\{R_0\, l^{-1/2}+a^{-1/2}\ln\frac{2ar_{\min}+b}{2(al)^{1/2}+2aR_0+b}\right\}. \tag{2.12}$$

Here τ^{-1} is the "knocking frequency" of the positron in the bound region $r \leqq r_{\min}$:

$$\tau=2\int_0^{r_{\min}} m/p\,dr=2\hbar(mc^2)^{1/2}/(\hbar c)$$
$$\cdot\left\{R_0^2\, l^{-1/2}-l^{1/2}/a-b\,a^{-3/2}/2\ln\frac{2ar_{\min}+b}{2(al)^{1/2}+2aR_0+b}\right\}. \tag{2.13}$$

The last two terms in $\partial\phi/\partial E$ result from the energy dependence of the effective potential.
When E_1 approaches $-mc^2$ the outer turning point $r_{\max}$ goes to infinity and Γ_1 vanishes exponentially [13]. The width increases with $|E_1|$ despite the increasing barrier height, because the tunneling distance $r_{\max}-r_{\min}$ becomes smaller. In Figure 2 the width $\Gamma_1(Z)$ is plotted. For comparison, energy and width of the $1s_{1/2}$ state calculated from a modified effective potential U_s [3] are also shown. This potential contains a centrifugal term

$$U_s=U+(\hbar c)^2/(2mc^2r^2) \tag{2.14}$$

which appears if the $1/r$ terms in the Dirac equation (2.2) are treated as if they were of zero order in $\hbar$ [14]. The modification leads to a third turning point r_1, with $0<r_1<R_0$. The eigenvalue equation is similar to (2.10), where $n=0, 1, 2, \ldots$ is now the radial quantum number. It follows from (2.2) that the centrifugal term may be important if the small component is dominant.
It turns out that the K-shell energy obtained with (2.14) decreases faster with Z than predicted in the literature [5, 10]. This is a hint to omit, as we have done, the centrifugal term for $s_{1/2}$ states. The WKB energy obtained from (2.10) lies above the energy calculated by Greiner and coworkers and below the value found by Popov. The width is by a factor of ≈ 3 larger than Greiner's result.

3. Spontaneous Positron Emission During the Ion-Atom Collision

In an adiabatic collision the time dependent molecular potential causes the electronic $1s\sigma_g$ state to change with time. Whenever the distance R of the two nuclei is less than R_{cr}, the distance at which the $1s\sigma_g$ state dives into the negative continuum, the quasibound positron (electron hole) can escape to an unbound continuum state. We do not touch the delicate question of how to produce the hole in the K-shell. If the hole is generated at the beginning of the collision it will in general live long enough to survive the collision. In the following we assume a hole to be in the $1s\sigma_g$ state during the collision, and we treat the decay in perturbation theory.

The probability for the spontaneous emission of a positron with fixed energy $|E_i|$ is given by the tunneling probability per unit time multiplied by the interval of time dt in which the energy $E_f(t)$ of the quasibound $1s\sigma_g$ state coincides with E_i [8]. The differential cross section is

$$\frac{d\sigma}{d|E_i|} = 2\pi \int_0^{b_{max}} b\,db\, 2\Gamma_1(E_i)/\hbar \left|\frac{dt}{dE_f}\right|_{E_i}. \quad (3.1)$$

The integration over the impact parameters b is restricted to close collisions. At $b = b_{max}$, the distance of closest approach $R_0(b)$ equals R_{cr}, and trajectories with $b > b_{max}$ do not contribute to the spontaneous positron emission.

Taking into account the finite width of the quasibound state and approximating its energy distribution by a gaussian with width $\Delta = \Gamma_1(E_f(t), t)/2$ we find

$$\frac{d\sigma}{d|E_i|} = 2\pi \int_0^{b_{max}} b\,db \int_{-\infty}^{+\infty} dt\, \Gamma_1(E_i, t)$$
$$\cdot \exp[-(E_i - E_f(t))^2/\Delta^2]/(\hbar\pi^{1/2}\Delta). \quad (3.2)$$

The normalization is chosen in such a way that we obtain (3.1) in the limit $\Delta \to 0$.

Near the turning point the energy $E_f(t)$ depends almost linearly on $R(t)$ [7]. We therefore take

$$E_f(R) = E_u + R\Delta E/\Delta R \quad (3.3)$$

where E_u is the K-shell energy of the united atom with $Z = Z_P + Z_T$. The other two quantities are

$$\Delta E = -mc^2 - E_u \quad \text{and} \quad \Delta R = R_{cr}.$$

We expand $R(t)$ around the turning point of the Rutherford orbit with impact parameter b:

$$R(t) = R_0(b) + R_1(b)\, t^2. \quad (3.4)$$

The constants R_0 and R_1 depend on the parameters of the internuclear orbit.

The decay width Γ_1 is a function of energy and of the time dependent nuclear two-center potential. Since R_{cr} lies inside the K-shell radius of the united atom, we approximate the two-center potential by its monopole term [4] and we introduce a time dependent charge

$$V(R, r) = -Z(R)\, e^2/r. \quad (3.5)$$

Near the turning point a linear interpolation is possible

$$Z(R) = Z_P + Z_T - R\Delta Z/\Delta R \quad (3.6)$$

with $\Delta Z = Z_P + Z_T - Z_{cr}$ and $\Delta R = R_{cr}$.

Figure 3 shows the cross section (3.2) for spontaneous positron emission in a (U, U) collision. R_{cr} is chosen to be 34 fm. The cross section is peaked at $E_i \approx$

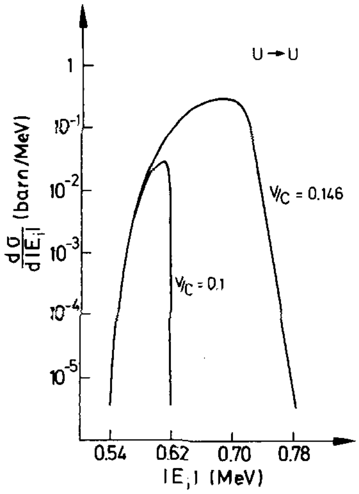

Fig. 3. Cross section for spontaneous positron production per vacancy for a (U, U) collision at two different projectile velocities

$E_f(R_0(0))$ because the region near the turning point is passed through slowly and also because the decay width increases with $|E_i|$. We find a strong increase of the cross section with projectile velocity v.

4. Induced Positron Emission

The time dependent molecular potential induces transitions from the quasibound $1s\sigma_g$ state into continuum states with a different energy [9]. An adiabatic basis will be used because the ion velocity is much smaller than the orbital velocity of the quasibound state. The exact time dependent solution of the Dirac equation ψ with its radial part $\binom{F}{G}$ can be expanded in terms of the stationary solutions $\psi_n(R)$ which depend on the internuclear distance $R(t)$:

$$\psi(t) = \sum_n A_n(t)\, \psi_n(R) \exp\left(-i\hbar^{-1} \int_0^t E_n(t')\, dt'\right). \quad (4.1)$$

In first order perturbation theory the amplitude for the transition into a continuum state with fixed energy E_i is given by

$$A_{fi} = -\int_{-\infty}^{+\infty} dt \exp\left[i\hbar^{-1} \int_0^t dt'(E_f(t') - E_i)\right]$$
$$\cdot \left[\langle F_f(R)| \frac{\partial}{\partial t} |F_i(R)\rangle + \langle G_f(R)| \frac{\partial}{\partial t} |G_i(R)\rangle\right]. \quad (4.2)$$

In the energy exponent we omit the imaginary part $\Gamma_1/2$ of the bound state energy E_f. In the case of (U, U) collisions this decay term would only lead to a correction of the order of $< 10^{-2}$. For $E_f \neq E_i$ the transition operator can be written

$$\frac{\partial}{\partial t}=-\frac{\partial V}{\partial t}\Big/(E_f(t)-E_i). \qquad (4.3)$$

We next evaluate the time integral (4.2) by contour integration. The poles are given by the zeros of $E_f(t)-E_i$. Bearing (3.3) and (3.4) in mind, level crossing will occur at

$$t=\pm t_0=\pm[(E_i-E_u-R_0(b)\,\Delta E/\Delta R)\,\Delta R/(\Delta E\,R_1(b))]^{1/2}. \qquad (4.4)$$

In the classically forbidden region, $E_i<E_f(R_0(b))$, t_0 is imaginary. For large values of $|t|$ the argument of the exponent in (4.2) behaves like $i(E_f(\infty)-E_i)\,t/\hbar$ where $E_f(\infty)$ is the $1s_{1/2}$ energy of the target (for $Z_T\geqq Z_P$). Therefore, one can close the contour (4.2) by a semicircle in the upper half plane and then calculate the residue at t_0. In the classically allowed region t_0 is real and we obtain half the sum of the residues at $t=\pm t_0$. Together with (3.5) we find

$$A_{fi}=-\int_{-\infty}^{+\infty} dt\,\exp\left[i\hbar^{-1}\int_0^t dt'(E_f(t')-E_i)\right]\frac{e^2\,dZ/dt}{E_f(t')-E_i}\,M$$
$$=-(e^2 M\,dZ/dt)_{t_0}\,i\pi\,S_0/t_0 \qquad (4.5)$$

with

$$S_0=\frac{\Delta R}{\Delta E\,R_1(b)}\cdot\begin{cases}\cos\left(\hbar^{-1}\int_0^{t_0}dt'(E_f(t')-E_i)\right), & t_0\text{ real}\\ \exp\left(i\hbar^{-1}\int_0^{t_0}dt'(E_f(t')-E_i)\right), & t_0\text{ imaginary}\end{cases}$$

$M=M_F+M_G$ is the transition matrix element.

The integration over space will be performed by the saddle point method. For monopole transitions, the large component of the continuum state $|F_i\rangle$ is given by its s-wave part

$$|F_i\rangle=a_i(p_i c)^{-1/2}\sin(k_i r) \qquad (4.6)$$

with $p_i=\hbar k_i=(E_i^2-m^2c^4)^{1/2}/c$. It will turn out that the point of stationary phase lies outside the barrier where the plane wave approximation (4.6) holds. A possible phase shift for large r is of no consequence for the transition probability. By means of (2.4) and (4.6) we find for the contribution M_F of the large components

$$M_F=\langle F_f(R)|\,1/r\,|F_i(R)\rangle$$
$$=a_i/2(p_i c)^{-1/2}\int_0^\infty dr\,a_f(p_f c)^{-1/2}\,r^{-1}\cos\varphi(r) \qquad (4.7)$$

with $\varphi(r)=\hbar^{-1}\int_0^r p_f\,dr-k_i r$, and we considered only the slowly oscillating part of the integrand. We recall that the index f refers to the bound $1s_{1/2}$ state which gets filled while a positron escapes.

The phase $\varphi(r)$ is stationary at $p_f=\hbar k_i$ which means that the saddle point r_0 is given by

$$r_0=Z(R)\,e^2/(E_i-E_f(t)). \qquad (4.8)$$

It follows from (4.4) that $r_0(t_0)\gg r_{\max}$. This implies that for $t=t_0$ the main contribution to the transition matrix element comes from the outer region, if one bears in mind the orthogonality of initial and final state. The slowly varying part of the integrand in (4.7) is taken out of the integral at $r=r_0$. Expanding $\varphi(r)$ up to second order in $r-r_0$ we find, retaining the exponentially decreasing term only

$$M_F=a_i\,a_f/4(p_i c)^{-1}\exp(i\varphi(r_0))$$
$$\cdot[(1/2+C(x))+i(1/2+S(x))]/x \qquad (4.9)$$

with

$$x^2=\varphi''(r_0)\,r_0^2/\pi=Z(t_0)\,e^2/(\hbar c)\,|E_i|/(\pi p_i c). \qquad (4.10)$$

We note that x is independent of r_0. The transition matrix element (4.9) contains the tunneling amplitude because of

$$\mathrm{Im}(\varphi(r_0))=\hbar^{-1}\int_{r_{\min,f}}^{r_{\max,f}}|p_f|\,dr. \qquad (4.11)$$

This reflects the obvious fact that for induced positron emission the positron must also tunnel through the barrier as in the case of spontaneous emission. It is consistent with the semiclassical approximation to replace the Fresnel integrals C and S by their asymptotic values 1/2. In our case this is accurate to a few percent.

The small component G deviates from F only by a preexponential factor, and we obtain the same phase dependence of both matrix elements in (4.2).

The differential cross section is given by

$$d\sigma=2\pi\int b\,db\,|A_{fi}|^2\,d\mathbf{k}_i/(2\pi)^3. \qquad (4.12)$$

The integration over the direction of the emitted positron with energy $|E_i|$ is readily performed since A_{fi} is isotropic. Inserting (4.5), we find with (4.9) and (2.5)

$$\frac{d\sigma}{d|E_i|}=e^2/(\hbar c)\,Z^{-1}\,\pi^2/8(E_i^2-m^2c^4)/(\hbar c)$$
$$\cdot\int b\,db\,|N_{if}(dZ/dR\,dR/dt)_{t_0}\,S_0\,T_i/t_0|^2. \qquad (4.13)$$

The normalization factor is given by

$$N_{if}=a_i\,a_f(p_i c)^{-1}(1+(E_i-mc^2)/(E_i+mc^2)) \qquad (4.14)$$

where a_f is obtained from the condition that, in the interior of the potential well, the final continuum

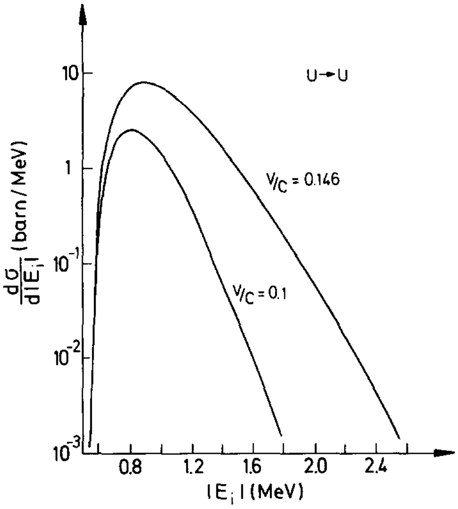

Fig. 4. Cross section for induced positron production per vacancy for a (U, U) collision at the same velocities as in Figure 3

function is normalized to one particle,

$$\int_0^{r_{\min}} dr(|F_f|^2+|G_f|^2)=1, \tag{4.15}$$

while the initial continuum function is normalized to plane waves. The last bracket on the right hand side of (4.14) contains an enhancement factor from the small component G. This factor almost cancels in N_{if} and we may approximate N_{if} by taking only the contribution from the large component F:

$$N_{if}=(4\pi\hbar c/k_i)^{1/2}(4mc^2/(c\tau))^{1/2}(p_i c)^{-1}. \tag{4.16}$$

The positron emission cross section is shown in Figure 4 in the case of (U, U) collisions. It vanishes exponentially at the threshold energy $|E_i|=mc^2$. The differential cross section increases with ion velocity v. The same is true for the total cross section for which we obtain 4 barn ($v/c=0.15$) and 1 barn ($v/c=0.1$) respectively. This is about one order of magnitude larger than the values obtained by Greiner and co-workers.

5. Conclusion

We have derived simple expressions for energy and width of the $1s_{1/2}$ state in a supercritical atom. The width is due to the tunneling of the vacuum electrons into the empty K-shell.

In the second part we considered spontaneous and induced positron emission. We showed how to treat the dynamic coupling between nuclear motion and electronic levels.

Within the semiclassical theory one finds the following. If the charge of the united system is smaller than the critical value 170 there is only induced positron emission. Its cross section is, however, very small and positrons with energies near the threshold mc^2 are favoured. When the united charge is overcritical and the internuclear distance smaller than R_{cr}, spontaneous positron emission becomes possible. While its differential cross section, $d\sigma_{sp}/d|E_i|$, is sharply peaked around the minimum energy of the quasibound $1s_{1/2}$ state, the cross section $d\sigma_{ind}/d|E_i|$ for induced positron emission is centered at much higher energies and has a very broad peak. In the case of (U, U) collisions the total cross section σ_{ind} is two orders of magnitude larger than σ_{sp} in agreement with Greiner's [9] result.

The cross sections given in this paper must be multiplied with the vacancy production probability for the K-shell to obtain the experimental yields. Preliminary estimates [16] of this vacancy production in very heavy-ion collisions yield very small probabilities ($\approx 10^{-5}$).

It has to be noted that pair creation will also originate from various background effects [6, 15]. Their mechanism does not require a K-shell vacancy.

A discussion of many-particle effects in supercritical atoms is far outside the scope of this work. Estimates may be found, for example, in Reference 3.

We are thankful to the Munich Tandem Group who directed our interest to this field.

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